Phase field modeling of interfacial dynamics

Qiang Du
Department of Mathematics
Penn State University

PENNSTATE
CAM@PS

Collaborators

- **Longqing Chen, Zikui Liu and Padma Raghvan** (PSU), **Chris Wolverton** (Ford), **Steve Langer** (NIST)

  Microstructure evolution in superalloy

  MatCASE (NSF-DMR-ITR) and CCMD (NSF-IUCRC)

- **Chun Liu, Jian Zhang, Peng Yu, Margret Slattery, Jiakou Wang, Tianjiang Li, Manlin Li, Meghan Hentry, Rob Kunz, Cheng Dong and Susan Gilmor** (PSU) **Xiaoqiang Wang** (FSU), **Rolf Ryham** (Rice)

  Complex/biological fluids

  NSF-DMS, NSF-CISE

Outline

- Motivation (materials, biology, …)
- Derivation of phase field models
- Examples based on recent works
- Adaptive numerical algorithms

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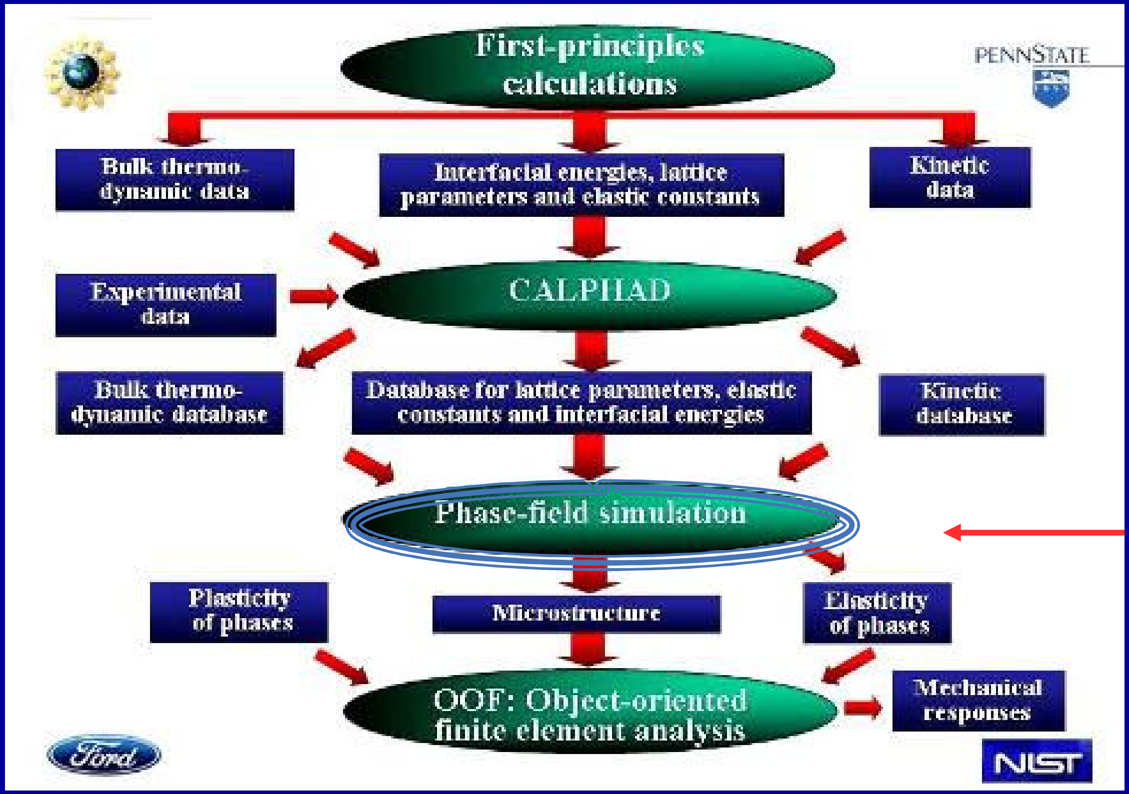
Motivation: MatCASE

http://matcase.psu.edu



Atomic structure

Microstructure evolution

grid enabled data intensive simulation tool

Liu-Chen-Raghavan-Du-Sofo-Langer-Wolverton, 2004: *An integrated Framework for multi-scale materials simulation and design,* J. Computer Aided Materials Design

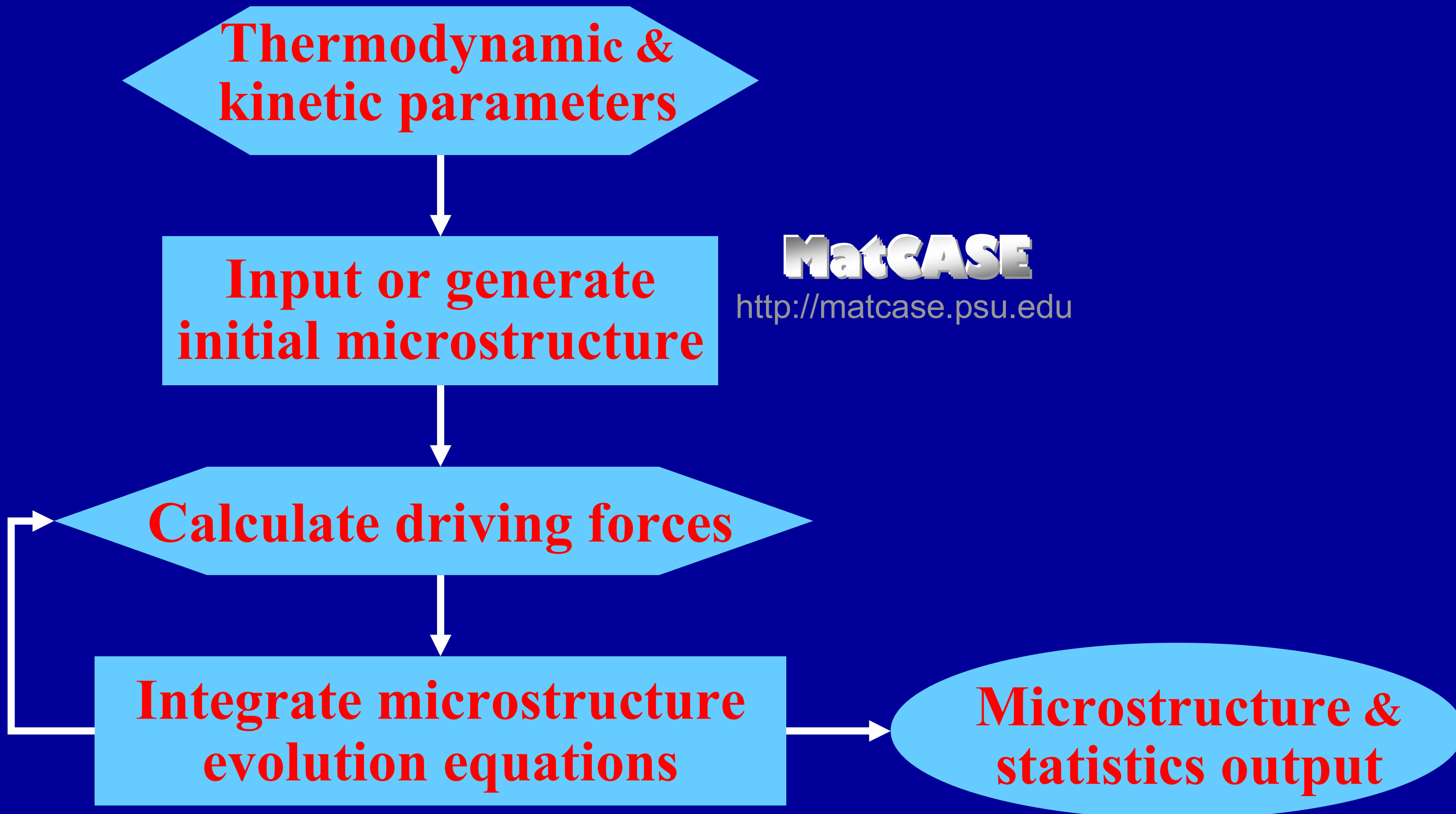
Phase Field/Diffuse Interface Modeling

- Popular for simulations of free and moving interface problems in materials sciences and other applications
- Sharp interfaces $\longrightarrow$ diffuse interfaces characterized by some phase field function

Eg: phase field simulations of microstructure evolution in ferroelectric thin films (Yu-Hu-Chen-Du, JCP 2005)

- Idea goes back to van de Waals,
  Ginzburg-Landau, Cahn-Hilliard, Halperin-Hohenberg, …

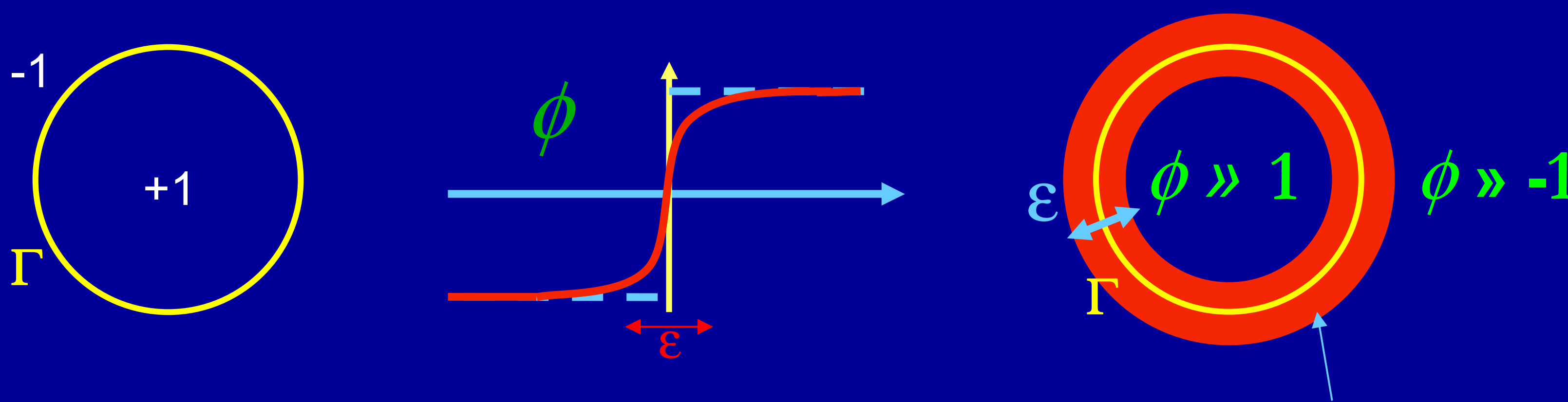
Phase-Field simulation of microstructure Evolution



MatCASE
http://matcase.psu.edu

Diffuse Interface/Phase Field

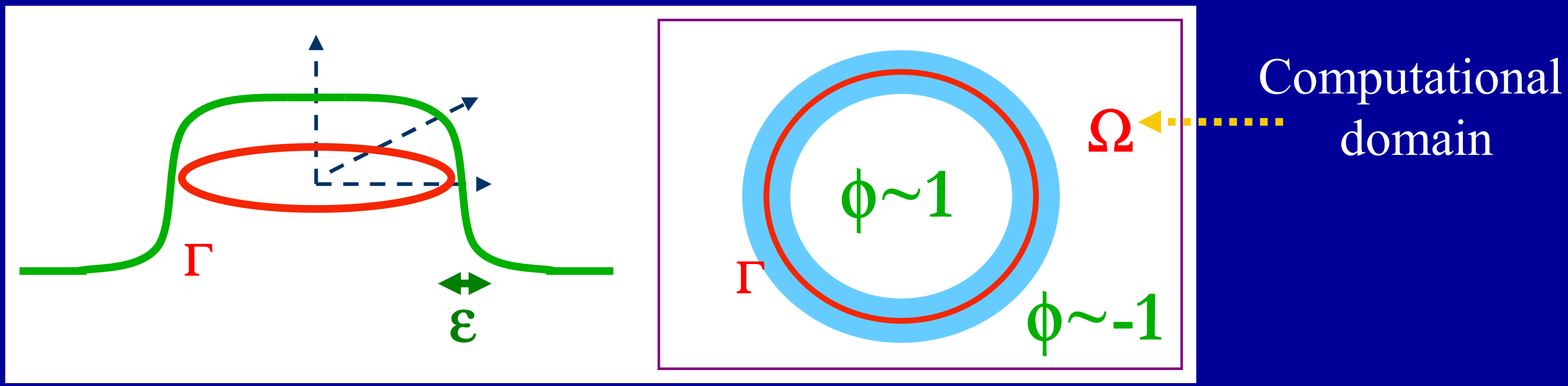
- **Geometric illustration:** introducing a smooth but nearly piecewise constant **phase field function ϕ** to label the two sides of the interface Γ.



- Interface Γ: zero level set of ϕ

Diffuse interface/Phase field

- How to describe the geometric features of Γ by ϕ?



Volume (difference) : $A(\phi) = \int_\Omega \phi \, dx$

Area: $B(\phi) = \int_\Omega \left(\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon} (\phi^2 - 1)^2 \right) dx$

(Cahn, Modica, Sternberg, Kohn, Gurtin, Chen, Evans-Souganidis-Soner…)

What about other geometric features, interfacial/bulk physics to be described in applications?

Case Study: Vesicle Membranes

Biomimetic cell membrane:
lipid vesicle

RBC

fluid bilayer formed
by amphiphilic lipids

Vesicle Membrane Models

- Atomistic models: *ab initio*, MD
- Coarse-grained models: MC, effective particle,
  triangulated networks, Browning dynamics
- Continnum mechanics:

  bending elasticity model for lipid bilayer

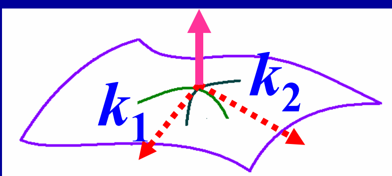
  (well-recognized, a good starting point)
- Multiscale models

Bending elasticity model

- **Earlier studies:** **Canhem 70, Helfrich 73, Evans 79, Fung, Lipowsky, Ouyang, Miao, Waugh, Iglic, Seifert, Wortis, Dobereiner, Chadwick , Gompper, Noguchi, Guven, …**
- **Hypothesis: vesicle Γ minimizes the bending elasticity energy s.t. volume/area constraints**

$$\textbf{min} \quad \mathbf{E} = \int_\Gamma H^2 ds$$

subj. to volume/area constraints



$$H = \frac{k_1 + k_2}{2}$$

mean curvature

Special case of Helfrich energy

$$\mathbf{E} = \int_\Gamma (a + b(H - c_0)^2 + cG) ds$$

Studies on Bending Elasticity Model

- **Analytical/geometrical constructions:**
  Helfrich, Lipowsky, Seifert, Wortis, Ouyang, Guven, …

- **Numerical simulations:**
  FEM, triangulated networks, surface evolver, moving LS, immersed boundary, lattice Boltzmann, particle dynamics…

- **Our recent works (JCP 2004, 2006, Nonlinearity 2005, SIAM Appl Math 2005, CPAA 2005, JCM 2006,) :**

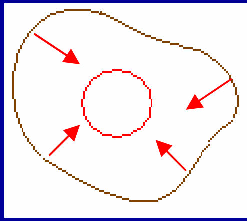
  Diffuse Interface/ Phase Field model

  energetic variational framework, no explicit surface tracking, allow complex topological changes, …

  Q: mean curvature of implicitly defined surface?

Phase Field Calculus

- **Geometric calculus:** variation of surface area/surface tension leads to mean curvature



- **Translate into Phase Field calculus:** variation of

$$\int_\Omega \left(\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2\right) dx$$ (area/surface tension)

gives the expression $-\epsilon\Delta\phi + \frac{1}{\epsilon}(1-\phi^2)\phi$

$$\boxed{\int_\Gamma H^2 ds} \longleftrightarrow \boxed{\frac{c}{\epsilon}\int_\Omega \left(\epsilon\Delta\phi + \frac{1}{\epsilon}(\phi^2-1)\phi\right)^2 dx}$$

- Similar extension to other features: spontaneous curvature, Gaussian curvature, ……, Du-Liu-Wamg JCP 04

Phase field bending elasticity model (PFBE)

Du-Liu-Wang JCP 2004

$$\min\ W(\phi) = \frac{c}{\epsilon}\int_\Omega \left(\epsilon\Delta\phi + \frac{1}{\epsilon}(\phi^2-1)\phi\right)^2 dx$$

$$\text{subject to } \int_\Omega \phi(x)\,dx = \alpha$$

$$\int_\Omega \left(\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2\right) dx = \beta$$

Vesicle Γ : zero level surface of the phase field function ϕ (enclosed in the computational domain Ω)

Dynamics: 1) gradient flow: $\longrightarrow$ $\dfrac{\partial\phi}{\partial t} = -\dfrac{\delta W_M}{\delta\phi}$

2) hydrodynamics

Sharp interface limit of PFBE $(\epsilon \to 0)$

- In Du-Liu-Ryham-Wang (Nonlinearity 2005), with ansatz

$$\phi(x) = q(y) + \epsilon h(x) + O(\epsilon^2) + \dots ,$$

it was shown

$$\phi(x) = tanh(\frac{y}{\sqrt{2}}) + O(\epsilon^2),$$

$$E(\phi) \to \int_\Gamma H^2 d\Gamma$$

$$y = \frac{d(x,\Gamma)}{\epsilon}$$

- Recently, by taking a more general ansatz

$$\phi(x) = q\,(y) + \epsilon h(y,x) + \epsilon^2 g(y,x) + \dots$$

Wang (2006) showed $q(y) = tanh(\frac{y}{\sqrt{2}}),\ \ h = 0,$

$$g(y,x) = r(x)s(y),\ E(\phi) \to \int_\Gamma H^2 d\Gamma$$

in addition, the variation $\longrightarrow$ Willmore stress

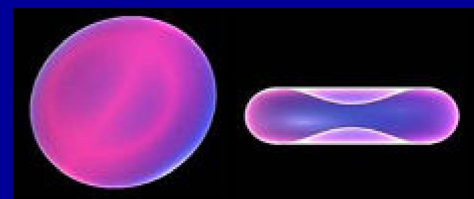
Minimum bending energy vesicles

Excess area:

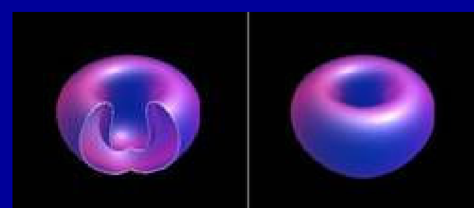
$$\sigma = \frac{\left(\frac{A}{4\pi}\right)^{1/2}}{\left(\frac{3}{4V\pi}\right)^{1/3}}$$

σ = 1 sphere

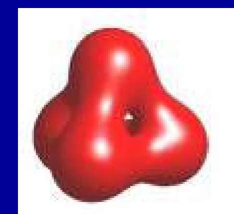
σ > 1 ?



discocytes

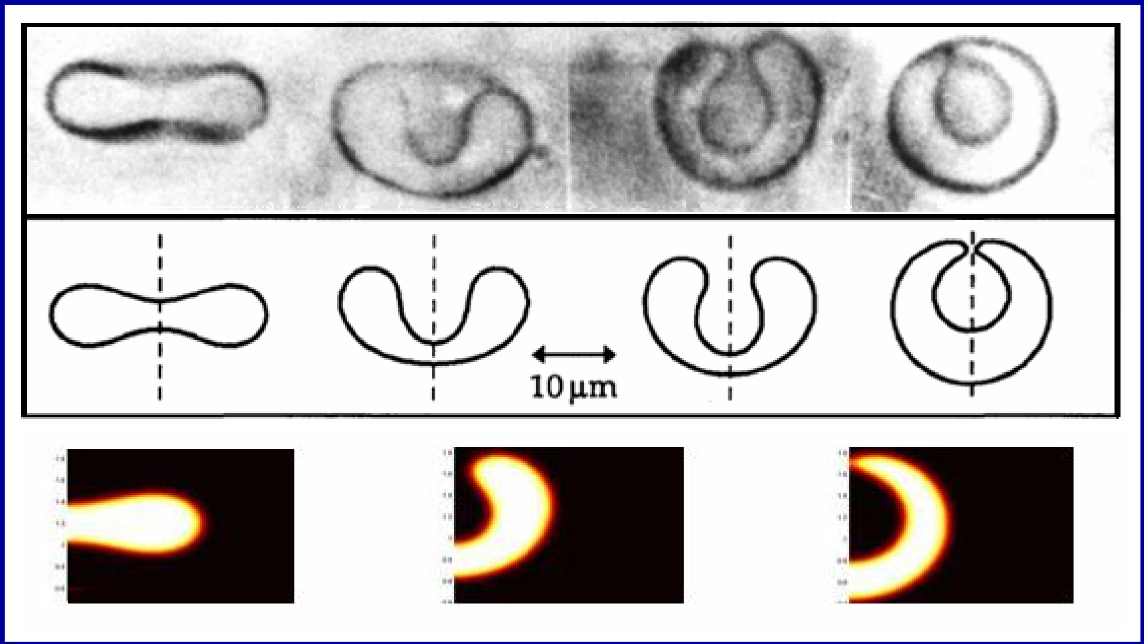


stomatocytes



Simulation vs. Experiment

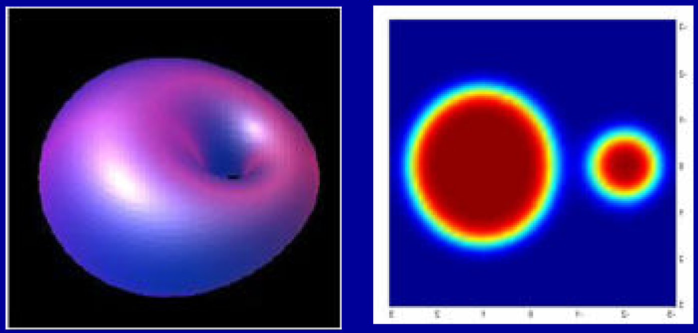
Berndl 1990: vesicle deformation in response to changing temperature **43.8-44.1°C**



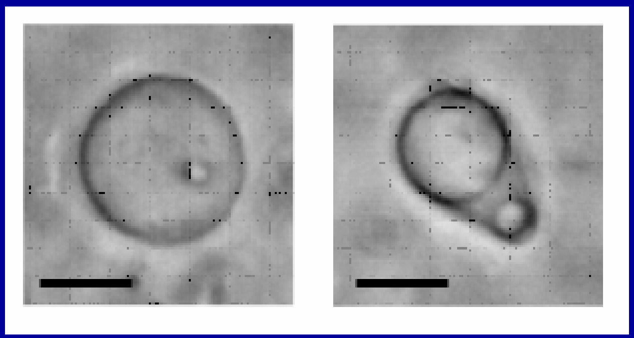
cross sections of 3d vesicles (Du-Liu-Wang JCP 2004)

Simulation vs. Experiment

- **Symmetric and non-symmetric torus (full 3d)**



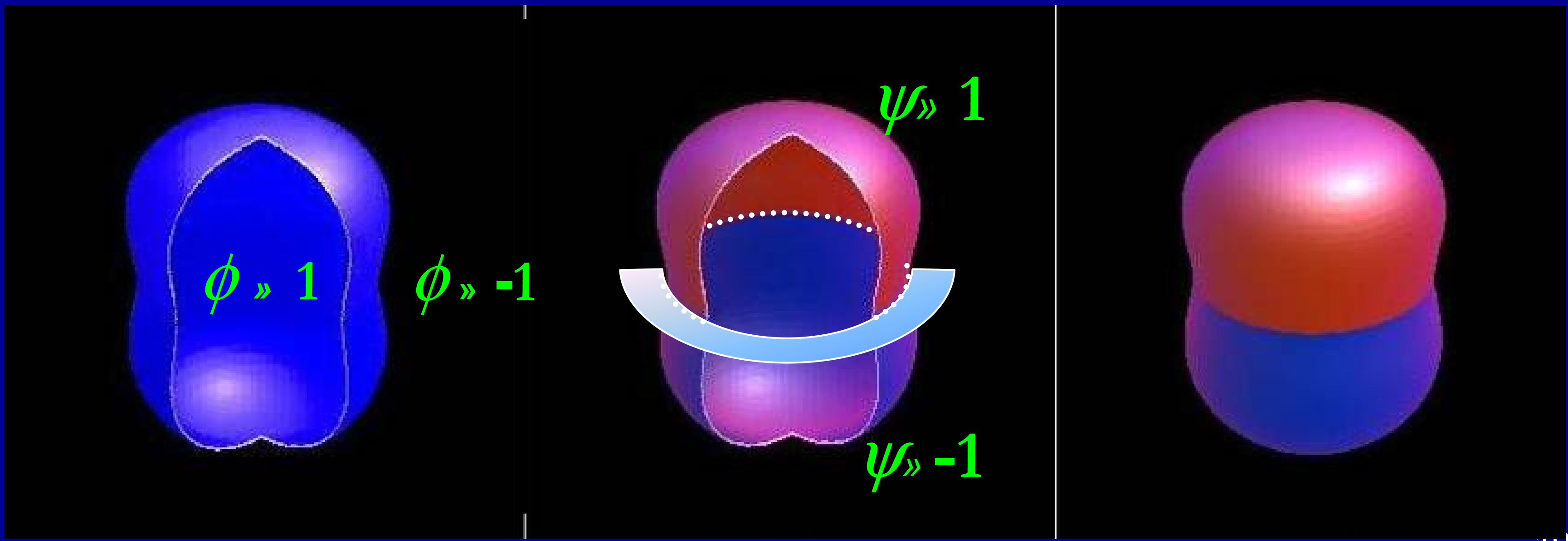
Du-Liu-Wang, J Comp Phys 2006



Michalet-Bensimon
Theory of Ou-Yang

Multi-component vesicles

- **Recent experimental studies of multicomponent membranes revealed intricate structure of rafts which are important for biological functions**
- **Phase field description of phase separation on a deformable membrane: multiple phase field functions + bending energy of membrane + line tension between different phases**



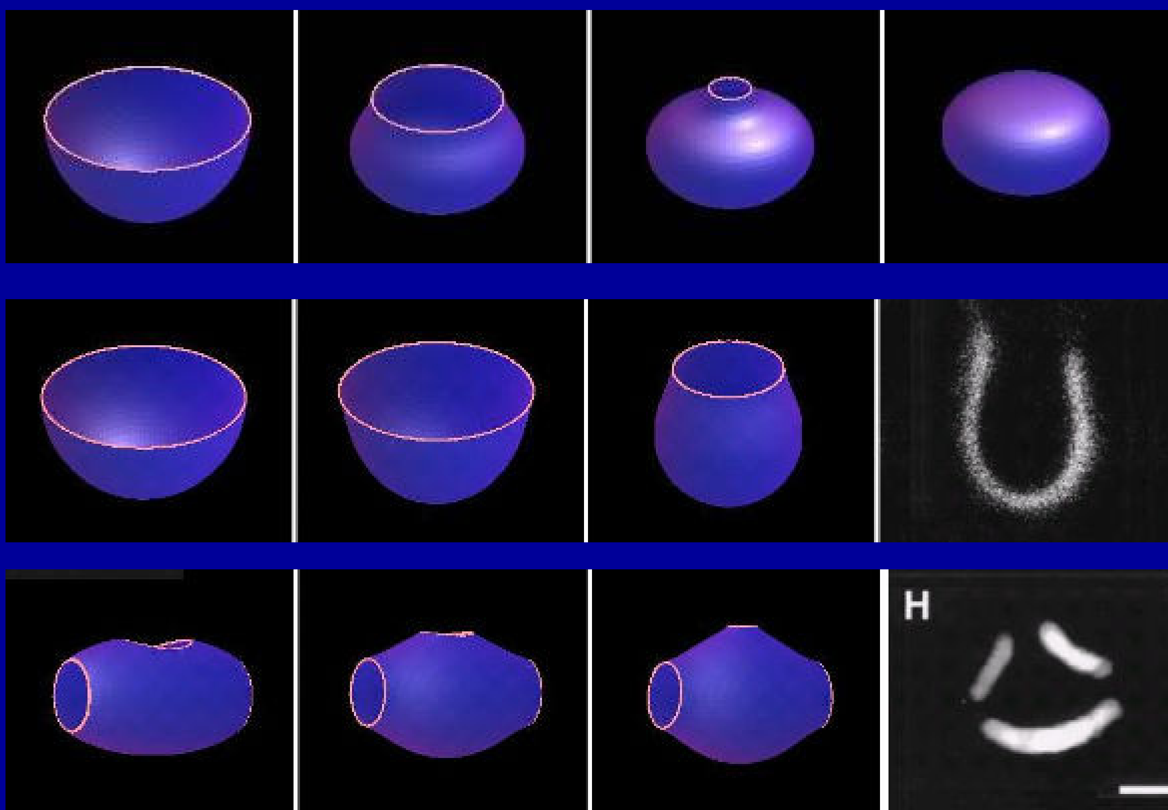
Modeling multi-component membranes

- **Wang-Du 2006: Phase field model for multicomponent vesicle with bending elastic energy + line tensions + fixed total volume + fixed surface areas for individual phases**
- **Simulation of vesicle phase separation: raft, microdomain**

Comparing our simulation with experiment (Baumgart et al, Nature 2003)

Similar extension: membrane with free edges

- Treat as a two-component membrane, pick bending rigidity to be zero in one component (Wang-Du 2006)



Saitoh-Takiguchi-Tanaka-Hotani

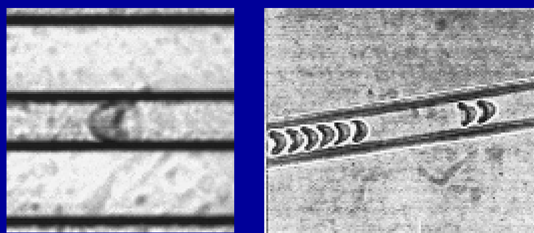
Capovilla-Guven-Santiago

Umeda-Suezaki-Takiguchi-Hotani

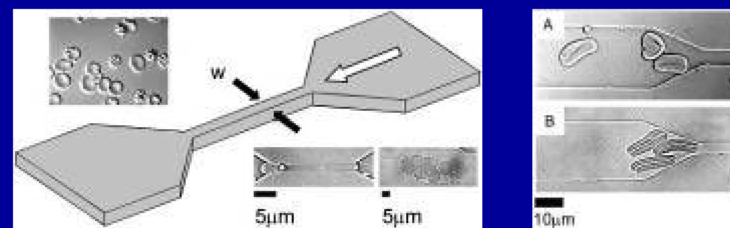
Ouyang-Tu

Phase field for interfaces in fluid

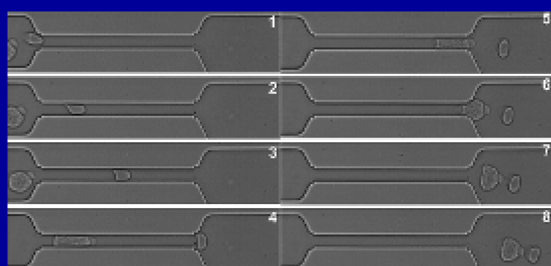
- **Experimental works on RBCs/vesicles in fluid**



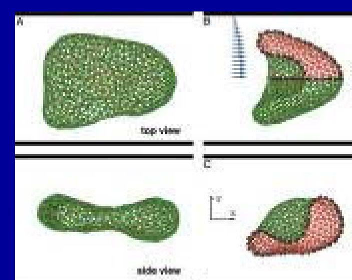
Tsukada et al 2001



Shelby et al 2003



Abkarian-Faivre-Stone 2006



Noguchi-Gompper 2005

- **Modeling/simulations**

Keller, Lipowsky, Pozrikidis, Grompper, Noguchi, Seifert, DeHaas, Misbah, Kantsler, WK Liu, Suresh

Phase-Field Navier-Stokes Model

Du-Liu-Ryham-Wang 2005

Membrane
Elastic
bending

transport

Willmore stress

Fluid
Incompressible
viscous

Phase field
Allen-Cahn/Cahn-Hilliard
fluid transport

$$\phi_t + u\nabla\phi$$

+

Navier-Stokes

Willmore stress

$$E'(\phi)\nabla\phi$$

A coupled vesicle/fluid model: PFNS

$$\begin{cases} \mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mu\Delta\mathbf{u} + E'(\phi)\nabla\phi, \\ \nabla\cdot\mathbf{u} = 0, \\ \phi_t + \mathbf{u}\cdot\nabla\phi = -AE'(\phi), \quad (A = -\Delta \text{ or } I \text{ or } 0\,) \end{cases}$$

Phase-Field
Navier-Stokes
(PFNS)

$$\frac{d}{dt}\left(\int_\Omega \frac{1}{2}|\mathbf{u}|^2\,d\mathbf{x} + E(\phi)\right) = -\int_\Omega \mu|\nabla\mathbf{u}|^2 d\mathbf{x} - \int_\Omega E'(\phi)AE'(\phi)d\mathbf{x}$$

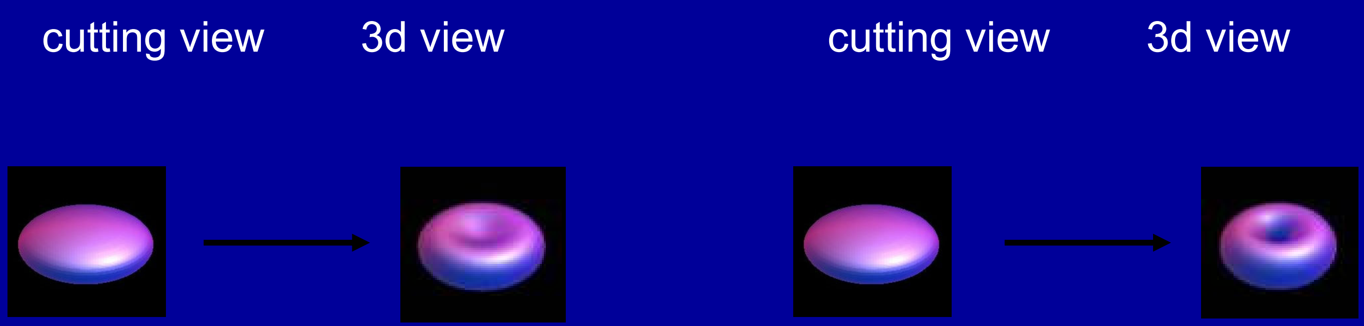
energy
law

Similar works: Siggia-Halperin-Hohenberg, Gurtin-Polignone-Vinals, Yue-Feng-Liu-Shen, Liu-Walkington, Lowengrub-Truskinovsky, Anderson-McFadden-Wheeler,… (note: **we use bending energy**)

Some examples

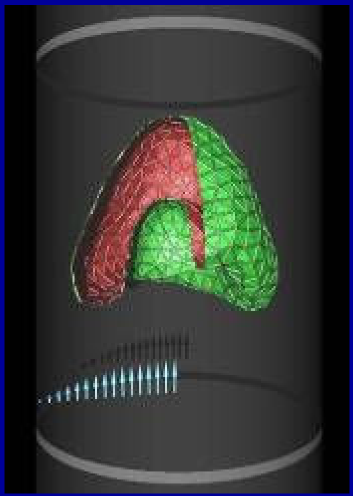
Du-Liu-Wang 2006

- Membrane/fluid interactions (single vesicle): fluid motion due to membrane deformation



Some examples

- Membrane fusion driven by fluid



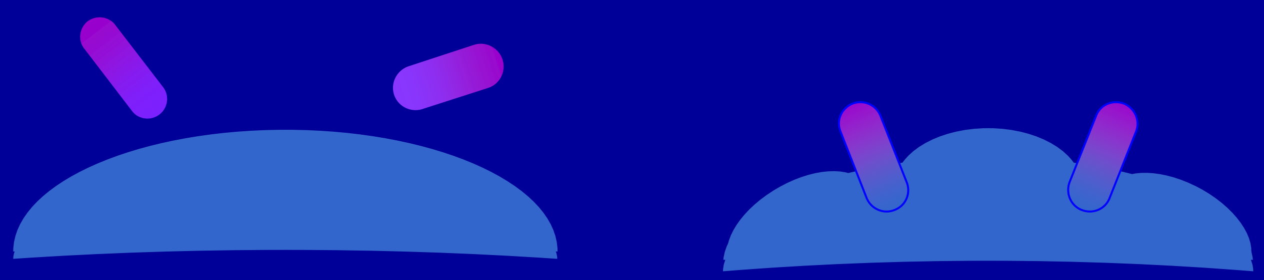
Noguchi-Gompper

cutting view

3d view

Extension: vesicle/protein interaction

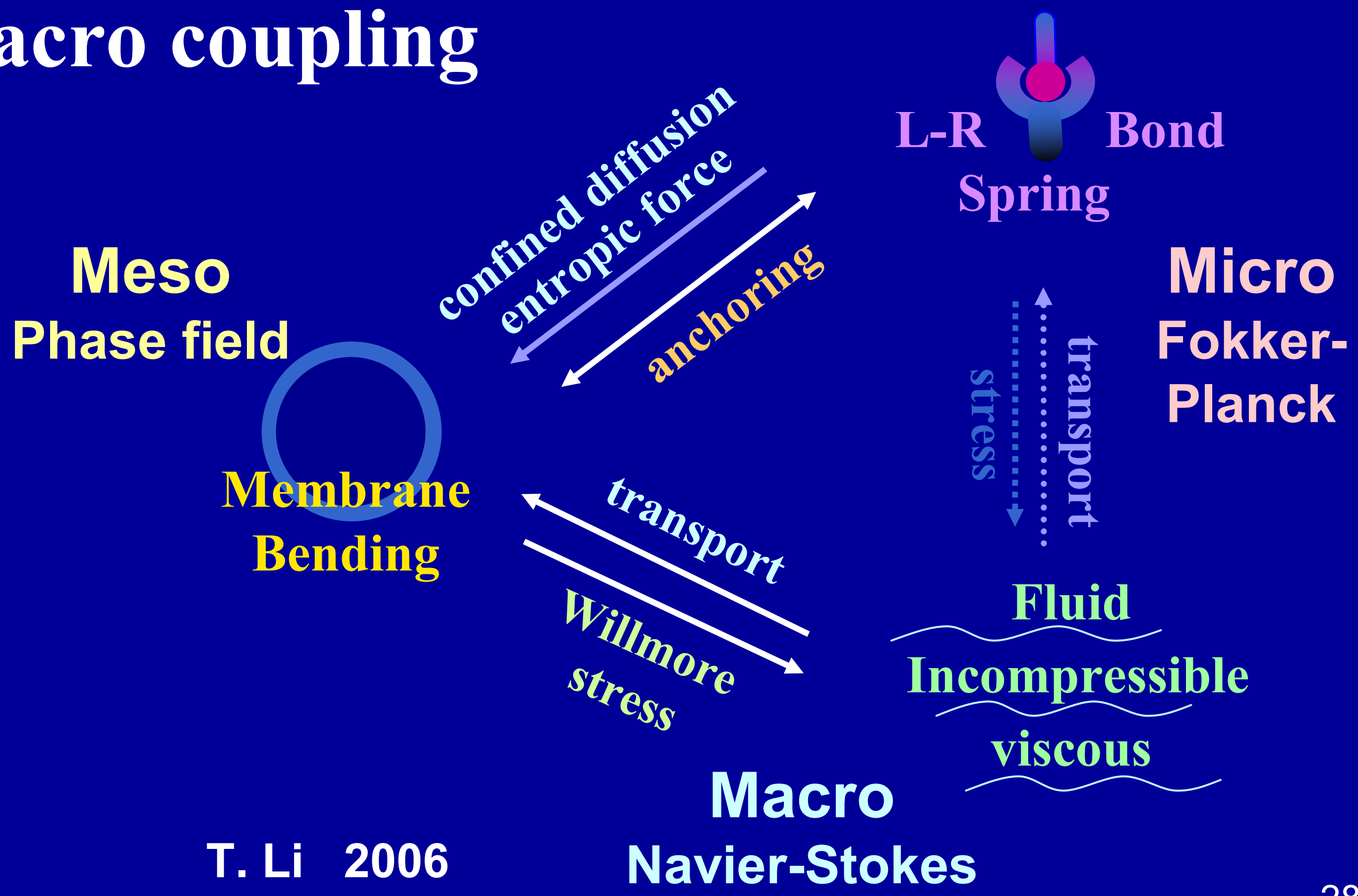
- **Vesicle mediated interaction (on-going): membrane deformation due to embedded proteins, which in turn determines the force and interaction between proteins**



- **Protein assisted vesicle fusion (on-going)**

Extension: protein + bilayer + fluid

- **Membrane adhesion (on-going): bonding between ligand-receptor ⟶ Multi-scale micro-macro coupling**



T. Li 2006

Phase Field/Diffuse Interface Modeling

- Simple, systematic derivation (geometry, energy, …)
- Interface capturing (no need for explicit tracking)
- Consistent to conventional sharp interface description
- Bridge effects from multiple scales/processes
- Effective for complex interfacial dynamics

efficient numerical algorithms !

Algorithms and numerical analysis

For Allen-Cahn, Cahn-Hilliard, Phase Field

- Finite difference, Finite element

  Fix/Lin, Caginalp/Lin, Elliott/French, Du/Nicolaides, Fife/Mackenny, Chen/Hoffmann, Wang/Sekerka, Feng/Prohl, Braun/Murray, Karma/Rappel, Provatas/Goldenfeld/Dantzig, Anderson/McFadden/Wheeler, Garcke/Nestler/Stoth, Mackenzie/Robertson, Wise/Lowengrub/Kim/Johnson, …

- Spectral/Semi-implicit

  Chen/Shen, Zhu/Chen, Liu/Shen, Yue/Feng/Liu/Shen

- Spectral/Exponential time difference (ETD)

  Du/Zhu (2004, 2005): FFT based, high order in both time/space

Recent development: adaptivity

- FEM for phase field bending elasticity model
  - mixed formulation, discrete energy-law preserving gradient flow, convergence analysis (Du-Wang, IJNAM)
  - nested saddle point formulation for mixed finite elements with optimal order error estimates (Du-L.Zhu, JCM)
  - full 3D adaptive FEM implementation based on residual type posterior error estimator (Du-Zhang, SISC)
- Spectral methods for phase field models
  - Applications to phase field bending elasticity model (Du-Liu-Wang, JCP)
  - Adaptive Fourier spectral via moving mesh method (Yu-Chen-Du, DCDS; Feng-Yu-Hu-Liu-Du-Chen, JCP)

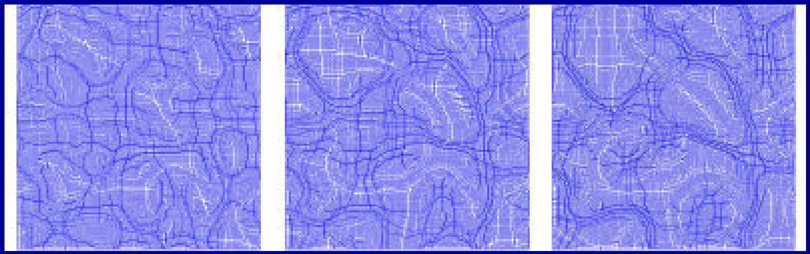
Spectral methods

Application to phase field models (Chen-Shen 92):

- **Phase field functions are smooth with given interfacial width**
- **Fourier Spectral: superior accuracy, fast implementation**
- **Rigid Cartesian grid structure**
- **Accuracy degradation if the interface is under resolved**

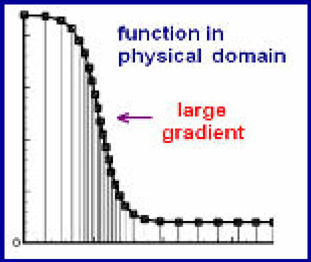
To better represent interfacial region

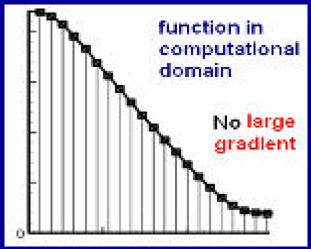
- **Moving mesh Fourier spectral (Yu-Du-Chen 2006, Feng-Yu-Hu-Liu-Du-Chen 2006):**
  following works of Winslow, Nakashashi-Deiwert, Bayliss-Kuske-Matkowsky, Huang-Ren-Russell, Ceniceros-Hou,…)

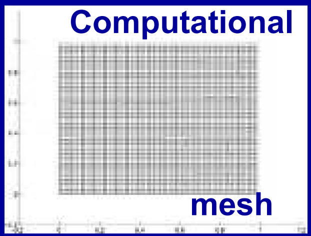


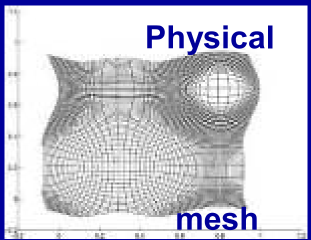
Moving Mesh/Fourier Spectral (MMFS)

(Feng-Yu-Hu-Liu-Du-Chen, JCP 2006)







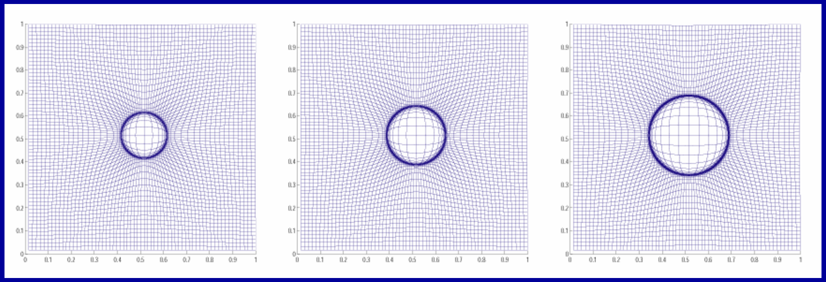


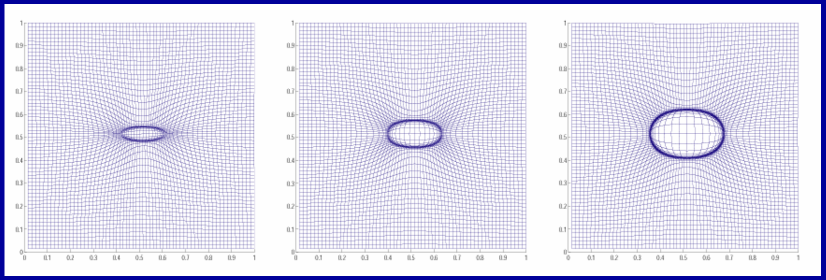
- **Large gradient in physical domain requires higher resolution, leading to prohibitively fine uniform mesh**
- **To make grids clustered near physical interface, a mapping is introduced between physical and computational domain so that the grids remain uniform in the latter**
- **MMFSM (moving mesh Fourier spectral method): mesh changes with solution to provide maximum resolution in physical domain**
- **Overcome variable coefficients due to mesh motion to allow FFT, reduce system size and improve accuracy**
- **Performance gain despite of the overhead**

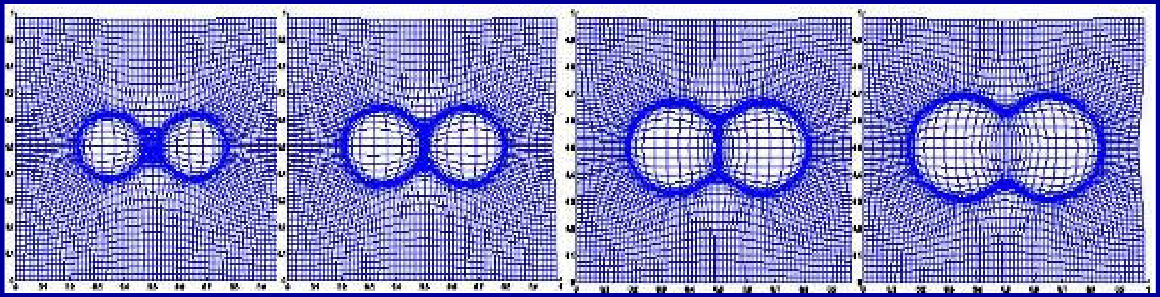
Moving Mesh/Fourier Spectral (MMFS)

- **Example:** **Application to Allen-Cahn model of microstructure evolution in a binary alloy**

(isotropic/anisotropic cases, Yu-Chen-Du 2006)

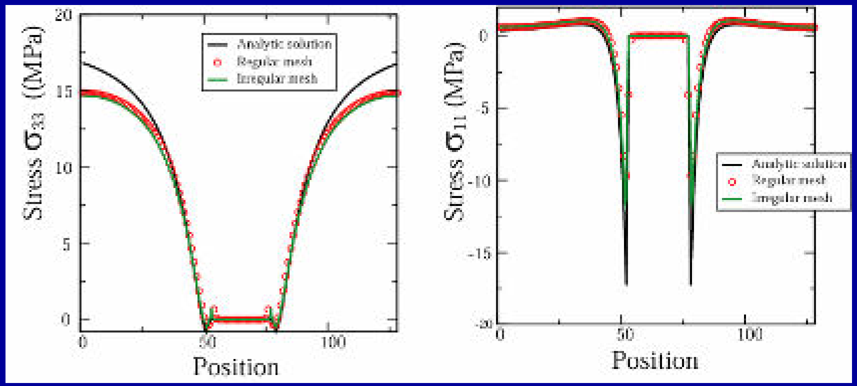


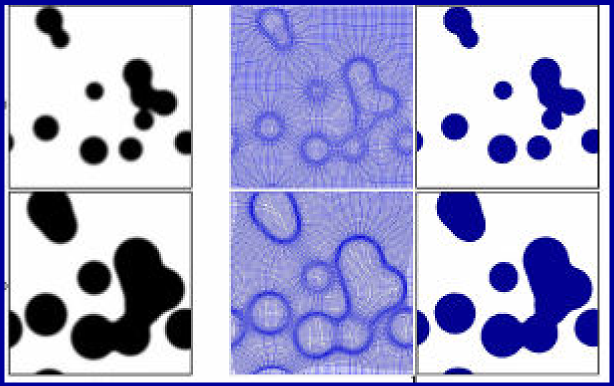




Moving Mesh/Fourier Spectral **(MMFS)**

- Two dimensional (Feng et al 2006)





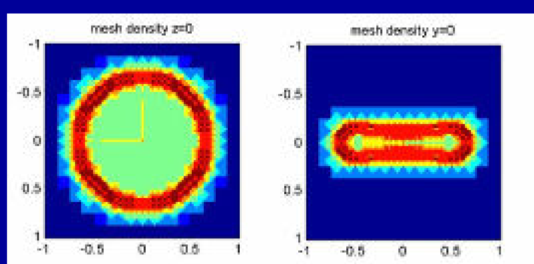
- Three dimensional (Feng et al 2006)

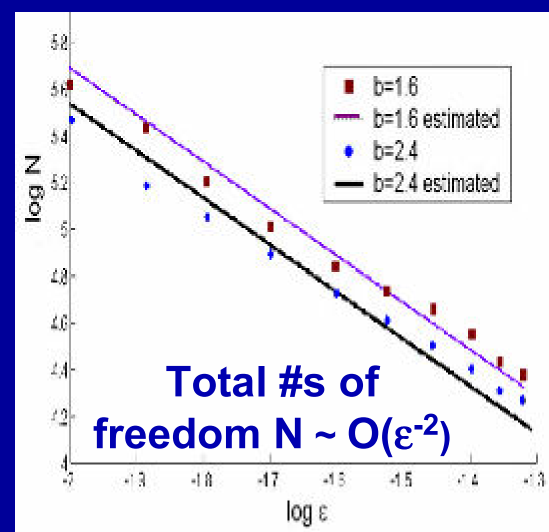
- Preliminary results demonstrate the effectiveness of MMFS

Adaptive 3d FEM

- **Vesicle membranes are 2-d surfaces, but phase field functions are solved in 3-d computational domain**
- **Adaptivity via residual a posteriori error estimates**
- **3D Computation gets reduced to 2D complexity**

mesh density

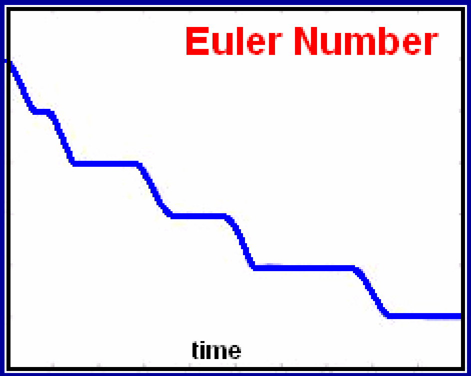




code developed by Jian Zhang, **anisotropic adaptivity?**

Automated topological information retrieval

- **Level-set/Phase field type methods are insensitive to topological changes (advantage or deficiency?)**
- **Formulae are developed to detect /control topology change in shape transformation via Euler number**



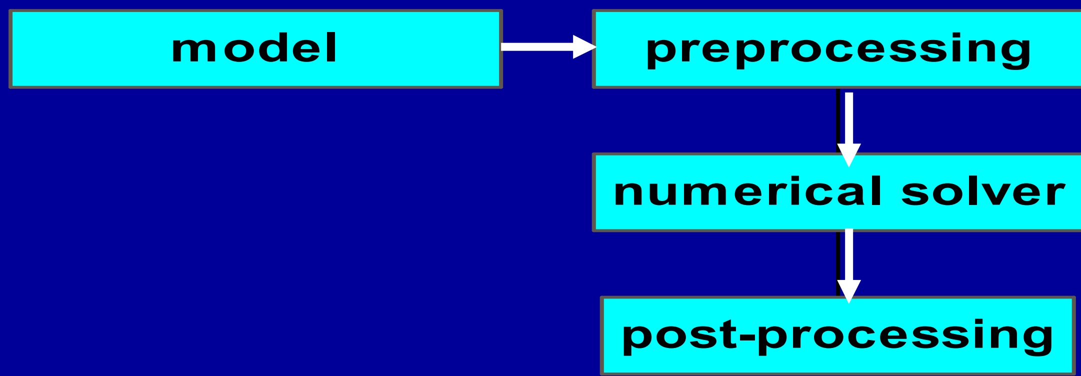
- **Connect geometry with topology, allow effective detection and control of topological events**

2d periodic: $$\chi = \frac{1}{4\pi\epsilon^2}\int_\Omega (\phi^2 - 1)\phi \, d\Omega$$

Du-Liu-Wang SIAM Appl Math 2005

A larger picture

- Computation in the traditional sense:



- The era of intelligent scientific computing:

find and simultaneously “recognize” the solution, discover new rules/principles

-- learning and knowledge discovery

Summary

- **Diffuse interface/Phase field model can be used to simulate many problems related to interfacial dynamics, and couple multi-scale, multi-processes**
- **Diffuse interface approach can be efficiently implemented via mesh adaptivity, and it is shown to be very effective through comparing with experimental findings**
- **Schemes for retrieving topological information within general diffuse interface framework may have broad applications**

Thank you!